

Mohamed M Aboelnga

List of Publications by Year in descending order

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105
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploring the structure function relationship of heme peroxidases: Molecular dynamics study on cytochrome c peroxidase variants. <i>Computers in Biology and Medicine</i> , 2022, 146, 105544.	7.0	3
2	Mechanistic insights into the chemistry of compound I formation in heme peroxidases: quantum chemical investigations of cytochrome <i>c</i> peroxidase. <i>RSC Advances</i> , 2022, 12, 15543-15554.	3.6	4
3	Comparative QM/MM study on the inhibition mechanism of \hat{I}^2 -Hydroxynorvaline to Threonyl-tRNA synthetase. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 115, 108224.	2.4	4
4	Acceptor Influence on Thiolate Sensing by Hemicyanine Dyes. <i>Journal of Organic Chemistry</i> , 2019, 84, 2261-2268.	3.2	13
5	Unveiling a Single-Metal-Mediated Phosphodiester Bond Cleavage Mechanism for Nucleic Acids: A Multiscale Computational Investigation of a Human DNA Repair Enzyme. <i>Journal of the American Chemical Society</i> , 2019, 141, 8646-8656.	13.7	33
6	Unraveling the Critical Role Played by $\text{Ado}^{\text{76}}\text{2OH}$ in the Post-Transfer Editing by Archaeal Threonyl-tRNA Synthetase. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1092-1101.	2.6	10
7	Roles of the Active Site Zn(II) and Residues in Substrate Discrimination by Threonyl-tRNA Synthetase: An MD and QM/MM Investigation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6163-6174.	2.6	8
8	A water-mediated and substrate-assisted aminoacylation mechanism in the discriminating aminoacyl-tRNA synthetase GlnRS and non-discriminating GluRS. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25598-25609.	2.8	12
9	Enzymatic Post-Transfer Editing Mechanism of <i>E. coli</i> Threonyl-tRNA Synthetase (ThrRS): A Molecular Dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) Investigation. <i>ACS Catalysis</i> , 2017, 7, 5180-5193.	11.2	9
10	Insights from molecular dynamics on substrate binding and effects of active site mutations in \hat{I}^{1} -pyrroline-5-carboxylate dehydrogenase. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1151-1162.	1.1	3
11	Substrate-Assisted and Enzymatic Pretransfer Editing of Nonstandard Amino Acids by Methionyl-tRNA Synthetase. <i>Biochemistry</i> , 2015, 54, 5757-5765.	2.5	11